

# DSMC Calculation of Supersonic Free Jets from an Orifice with Convex and Concave Corners

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**Abstract.** Supersonic free jets from an orifice with convex and concave corners are investigated in three-dimensional field by the DSMC method. The plumes develop faster from the concave corners of a hexagram orifice with symmetric cross section than those from the convex corners. The mechanism of the development is revealed through the observation of velocity vectors right behind the orifice. The directions of flow are also investigated in various cross sections of a jet. There is a complicated flow-field and several circulations of flow are observed. The variation of cross section of a star-shaped jet along the jet axis changes with the ratio of a stagnation pressure to a background pressure. In an asymmetric orifice, a plume from a concave corner is inclined to an adjacent plume and they are merged into a bigger plume.

## INTRODUCTION

Rarefied supersonic free jets through an orifice or a nozzle need to be studied in detail because these are applicable to the discharge of gas into a vacuum chamber or rocket propulsion in space. We have applied the direct simulation Monte Carlo (DSMC) method [1] to the structural analysis of free jets and we have shown that Mach disk and a barrel shock in a free jet can be reproduced by the molecular simulation [2]. We have also applied the DSMC method to an analysis of plume-plume interactions [3]. Thus, we are sure of the DSMC method being effective in research of a free jet. In three-dimensional calculation, however, since there exists many cells in flow-field, the number of molecules in a cell may be restricted very small and, in an extreme case, it becomes one or less. When being forced to use such a small number of molecules, its influence on results of a free jet should be examined in advance. In the present paper the effect of the number of molecules in a cell is investigated in case of an axially symmetric free jet. It is well known that the jet from non-axisymmetric orifices does not develop its cross section as the cross section of the orifice. Teshima [4] has made the experiments of supersonic expansion from polygonal orifices with convex and concave corners by the LIF experiment and shown the deformation of cross section of the jet from a hexagram orifice. While the change of jet cross section is applicable to promotion of gas mixing, the mechanism may depend on vortex motions in the plane normal to the jet axis. The analysis in detail has to rely only on a three-dimensional molecular simulation. In the present study the DSMC method is applied to the analysis of a free jet from an orifice with complicated cross sections. The plumes issuing from a hexagram orifice develop faster from the concave corners than those from the convex corners. The mechanism of the development is revealed through the observation of velocity vectors right behind the orifice. The directions of flow are also investigated in various cross sections of a jet. There is a complicated flow-field and several circulations of flow are observed. The variation of cross section of a jet along its axis also changes with the ratio of a stagnation pressure to a background pressure.

## CONDITIONS OF CALCULATION

Figure 1 shows the cross sections of star-shaped orifices, a symmetric hexagram (a) and an asymmetric one (b). The calculations are made under the conditions:  $1/Kn=2500$  and  $p_0/p_1=12.5, 50, 100$ , where  $Kn$  is the Knudsen

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number based on the mean free path at the upstream stagnation and the characteristic length which is an equivalent diameter  $d$  of hydrodynamics,  $p_0$  is the stagnation pressure, and  $p_1$  is the background pressure. The simulated domain is divided into two regions, upstream and downstream of the orifice. The typical size of upstream flow-field of the orifice is  $1.5d \times 1.5d \times 3d$ , and that of downstream is  $19.8d \times 6.3d \times 12.6d$ . The VHS molecular model [1] for a monatomic gas of argon is used. The temperature index of viscosity coefficient  $\omega$  at room temperature is adopted. The temperature of a free jet drops suddenly as the jet expands, but for a gas of a single species a constant value of the index is available in the simulation. The null-collision scheme [5] is used for intermolecular collisions. It is similar to the no-time-counter scheme [1] by Bird, both schemes belonging to the maximum collision number method, but it uses an instantaneous value  $N$  for the number of molecules in a cell in the calculation of the maximum collision number  $N(N-1)(\sigma_T c_r)_{max} \Delta t / 2V$ , where  $(\sigma_T c_r)_{max}$  is the maximum product of the total collision cross section  $\sigma_T$  and the relative speed  $c_r$ ,  $\Delta t$  is the time step over which the molecular motion and the intermolecular collisions are uncoupled, and  $V$  is the volume of a cell. This is in contrast with Bird's scheme in which the time average  $N_{av}$  instead of  $N-1$  is used, such as  $N_{av}N(\sigma_T c_r)_{max} \Delta t / 2V$ .

The diffusely reflecting surface of the orifice is assumed. Velocities of each molecule entering through the upstream boundary are generated using the Maxwell distribution with some flow velocity normal to the boundary. On the other hand, those of molecules entering through the downstream boundary (boundary normal or parallel to the axis in the downstream region) are generated by the Maxwellian at the background pressure without flow velocity. The maximum number of simulated molecules, dealt with simultaneously in a computer, is about  $2 \times 10^7$  and the maximum number of cells is about  $3 \times 10^7$ . That is, the average number of molecules per cell is 0.7. There is the question of whether a possible collision pair can be found in the cell that has only one molecule or less on average. The answer is that since the cell with one molecule on time average has occasionally no molecule at all as a statistical fluctuation, it must also have two or more molecules occasionally in order to keep one molecule on time average. The statistical proof that the average number of molecules which would seem insufficient reads to the theoretical collision rate correctly has been discussed [6]. The number of molecules per cell should be decreased in order that the total number of molecules does not exceed the permissible amount in the available computer system, especially in three-dimensional calculation. Furthermore, in the study of steady flow the process of an unsteady state before attainment of steady state can be calculated rapidly with a small number of molecules.

Before the three-dimensional simulation of a star-shaped jet, the DSMC results of a simple axisymmetric jet obtained with different number of molecules have been compared and discussed. In an axisymmetric jet, the minimum number of molecules per cell on time average occurs at the location directly before the Mach disk in the jet axis. Figures 2 and 3 indicate the density profiles  $\rho/\rho_0$  of jet flow-field (axially symmetric) for  $1/Kn=2500$  and  $p_0/p_1=50$  which are calculated with the dimensions of the cell located near the orifice being about 14 times the local mean free path, where  $\rho_0$  is the density at the upstream stagnation. Figure 2 is obtained using about  $5 \times 10^6$  molecules and the minimum number of molecules per cell is about one. On the other hand, Fig. 3 is obtained using about  $5 \times 10^5$  molecules, which is about one-tenth of the number of molecules in Fig. 2, and the minimum number of molecules is about 0.1. In Fig. 3, almost the same result as that in Fig. 2 is obtained except for the narrow area where the number of molecules per cell is less than 0.2, even if many cells near the jet axis have a very small number of molecules, less than one on time average, as in Fig. 4. The minimum number of molecules per cell being 0.7 need not be considered insufficient in the calculation for a free jet. The upstream cell network is constructed by square cells but, in the downstream, the dimensions of a cell along the axis vary exponentially with its position up to the location of the Mach disk since the minimum density appears immediately before this location.

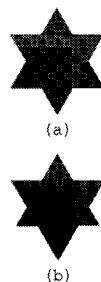


FIGURE 1. Cross sections of orifices (a) and (b).

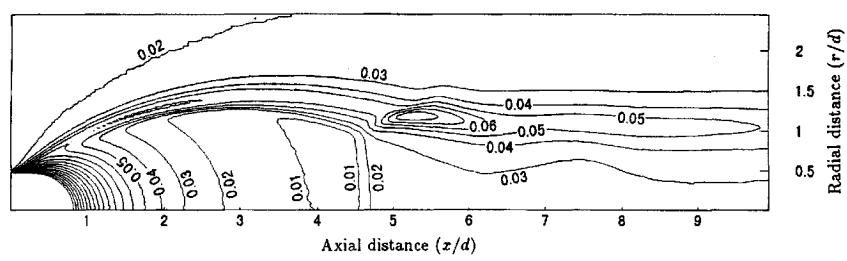


FIGURE 2. Contours of normalized density obtained using  $5 \times 10^6$  molecules ( $1/Kn=2500$ ,  $p_0/p_1=50$ ).

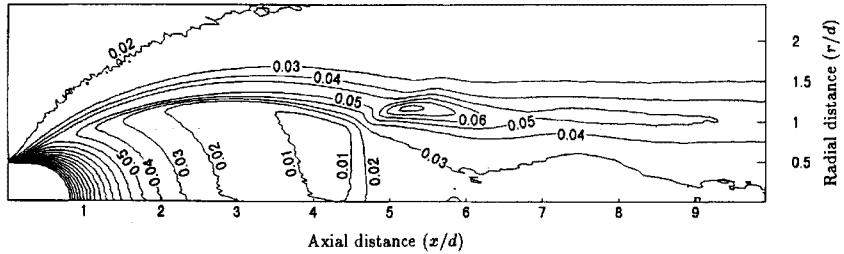


FIGURE 3. Contours of normalized density by small number of molecules ( $1/Kn=2500$ ,  $p_0/p_1=50$ ).

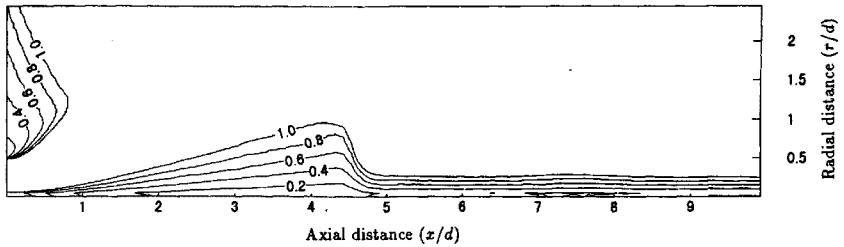


FIGURE 4. Number of molecules in each cell (Region less than 1.0).

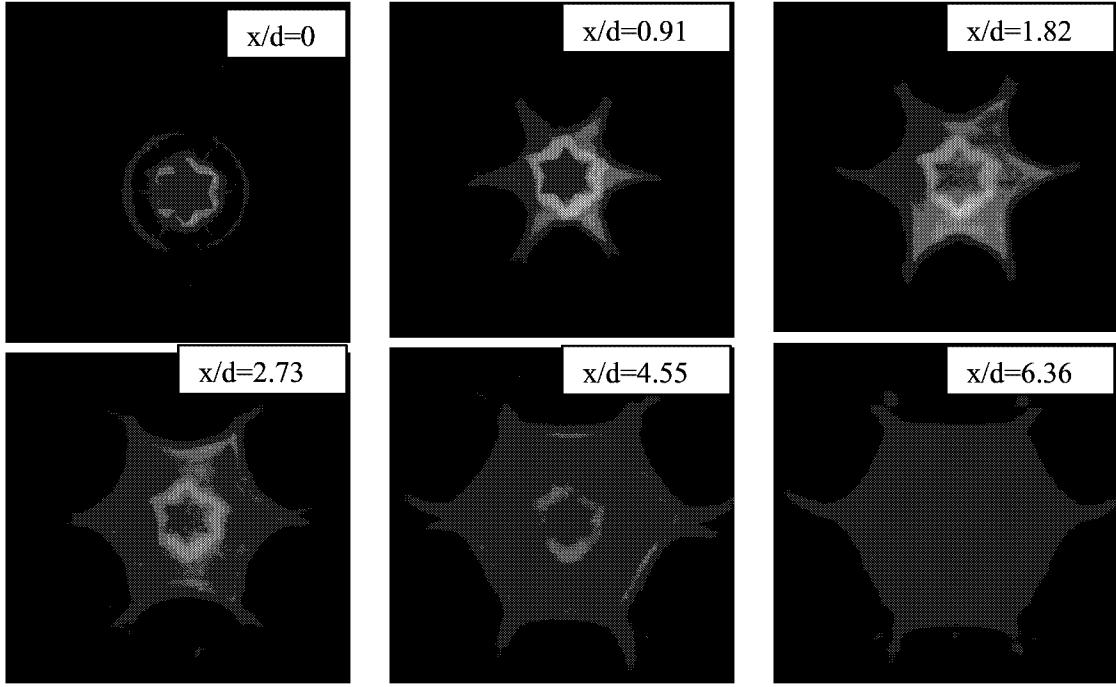
## RESULTS AND DISCUSSION

First, the DSMC calculation was compared with the experiment in the pressure ratio  $p_0/p_1=100$ . The result obtained by LIF (a laser induced fluorescence) experiment is shown in Fig.5. The equivalent diameter of an orifice is 2.2 mm. The stagnation pressure is 100 Torr and the background pressure is 1 Torr. Then, the pressure ratio is 100. Fig.6 shows the results of density distribution obtained by DSMC calculation in the condition of  $1/Kn=2500$  and  $p_0/p_1=100$ . They are normalized by the stagnation density. Both results (Figs. 5 and 6) are the density profiles on various planes perpendicular to a jet axis. The growth of jet plumes from the concave corners of an orifice is remarkable, and an outflow like a wheel of a carriage can be seen immediately after the exit of an orifice in the experiment. The density distribution of the same wheel form has been obtained also in the DSMC calculation. In the experiment, the free jet grows up to the star-shaped one with sharp tips, and turns into the jet of a hexagon. Moreover, thin jet streams blow off from the tips and they are swinging. On the other hand, although a star-shaped jet and a hexagon jet are also formed in the calculation, the thin jet streams from vertexes cannot be observed. It is considered as the reason that the present simulation uses too coarse cells to reproduce the detailed structure like the experiment.

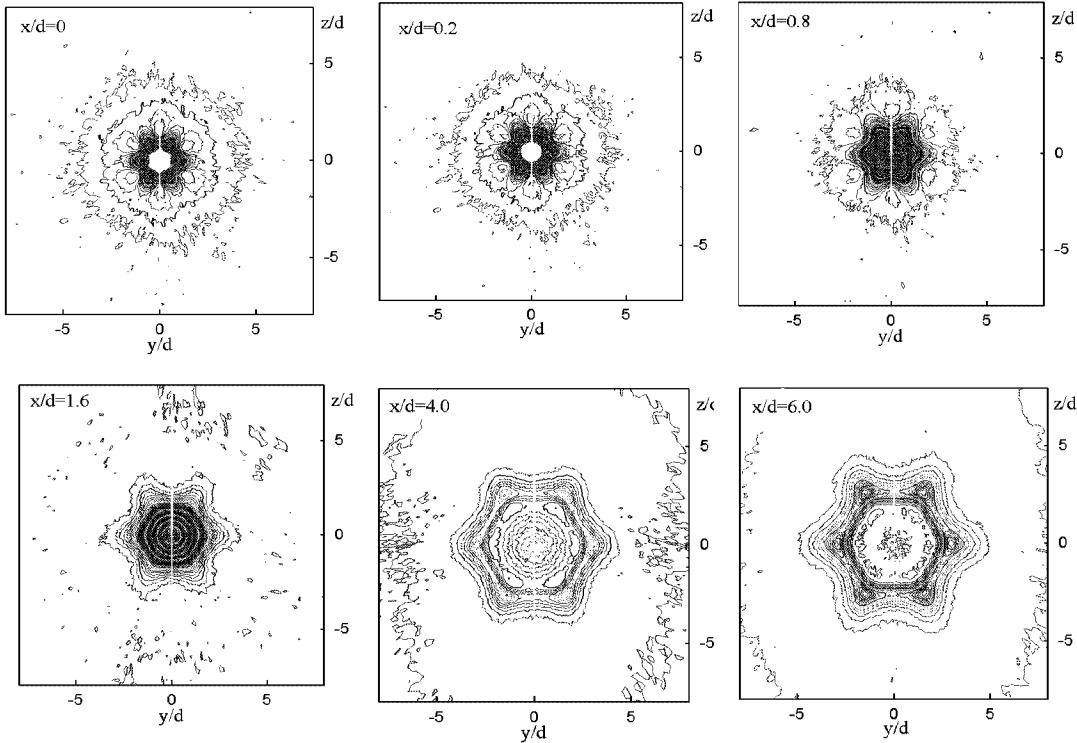
Figure 7 shows the density profiles obtained by the DSMC in 3-dimensional graph. It seems that the density of the vertex of a hexagon increases from  $x/d=3.0$  and, contrary to this, the density near a jet axis falls. Fig.8 draws Mach number profiles, velocity profiles of radial direction, and those of tangential direction. In the radial velocity an outward flow is regarded as positive and in the tangential velocity a counterclockwise rotation is taken as positive. Both velocities are normalized by the most probable molecular speed at stagnation temperature. Although a sharp change of a Mach number profile just behind an orifice can be seen, the comparatively quiet distribution is produced in the downstream from  $x/d=1.6$ . On the other hand, the velocity of radius direction has the tendency to take the local maximum in the root of arms of a star-shaped jet. Moreover, since the value is negative in the circumference of a jet, it turns out that the star-shaped jet is formed involving gas from the circumference. The phenomenon is also explained using the velocity vector diagram mentioned below. In addition, the counterclockwise flow in the right-hand side of the root of arms of the star-shaped jet is produced in the velocity profiles of tangential direction, and the clockwise flow in the left-hand side of it is produced. Namely, the gas flowing in from the circumference of a jet changes its direction at the root of a jet arm, and flows out along with the arm of a jet. This also becomes clear by the velocity vector diagram.

Figure 9 shows the density distributions that are obtained in the condition of the pressure ratio 50, maintaining the stagnation pressure constant. Compared with the pressure ratio 100, growth of arms of a star-shaped jet and also

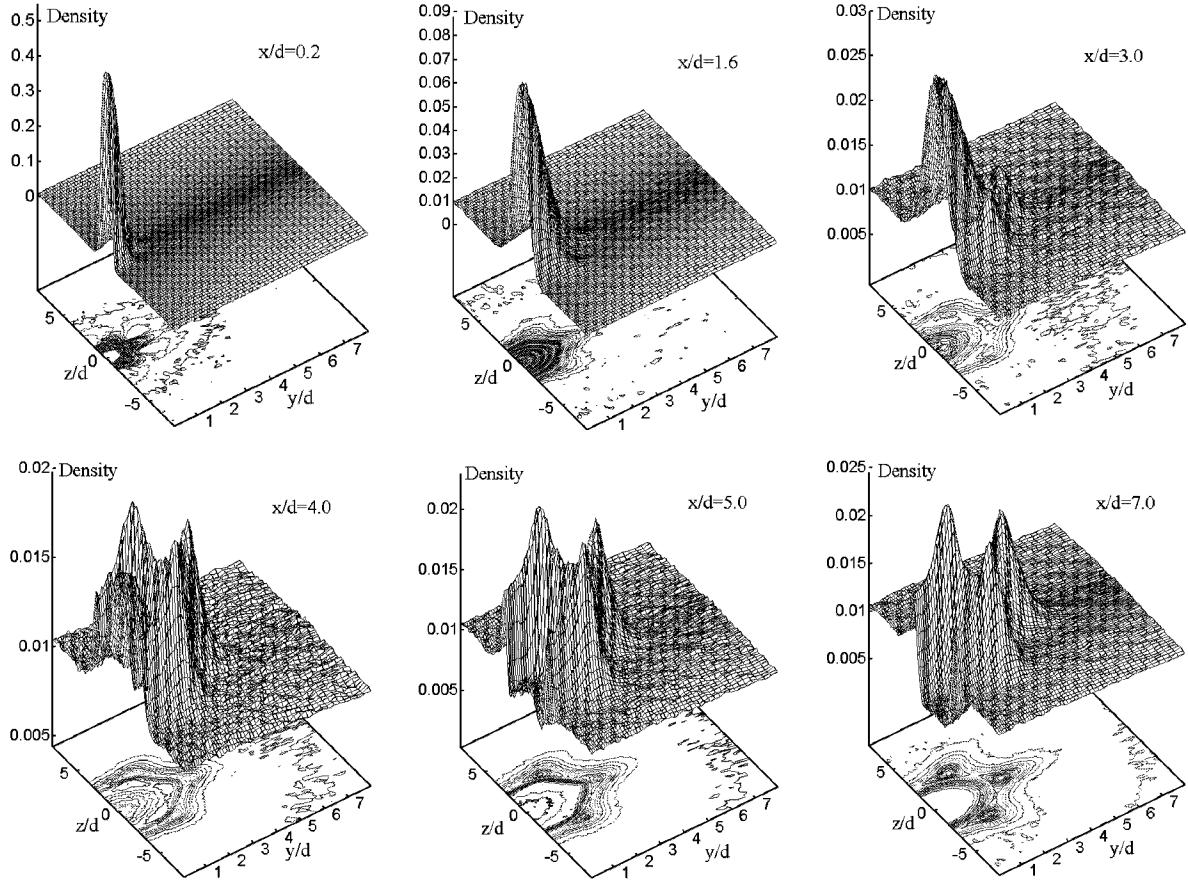
growth of the local maximum of the root of the arms become more remarkable. Although not shown in a figure, it was clarified that the growth of arms of a jet becomes blunt conversely in the calculation performed by the pressure ratio 12.5. The influence of a pressure ratio on the star-shaped jet should be investigated in more detail in the future.



**FIGURE 5.** Visualization using a laser induced fluorescence (LIF) technique.



**FIGURE 6.** Density contours obtained by the DSMC method ( $1/Kn=2500$ ,  $p_0/p_1=100$ ).



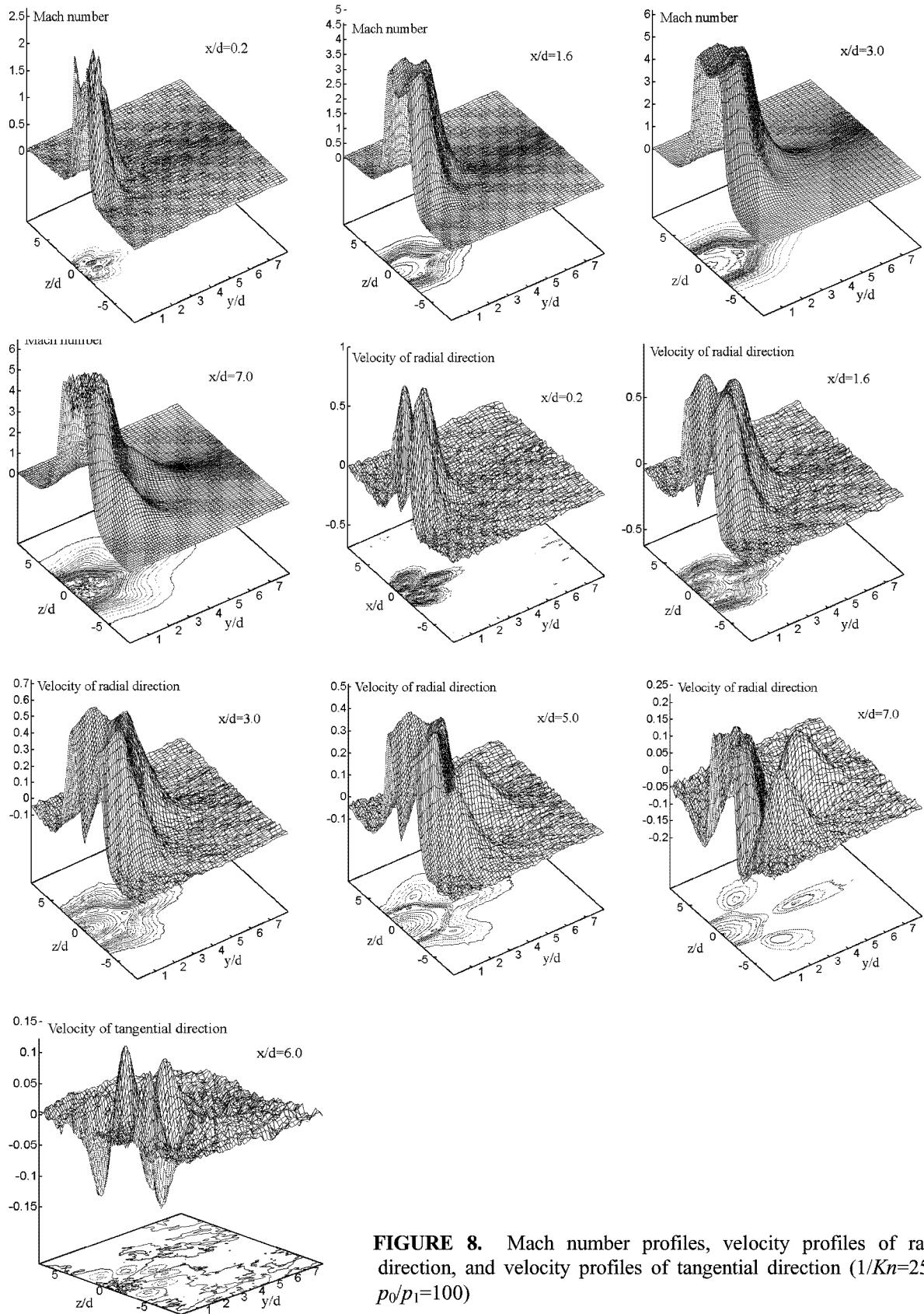
**FIGURE 7.** Density profiles by the DSMC method in 3-dimensional graph ( $1/Kn=2500$ ,  $p_0/p_1=100$ ).

Figure 10 shows the density contours in planes normal to the jet axis ( $1/Kn=2500$ ,  $p_0/p_1=50$ ), where the simulation domain is restricted to a half of the entire flow-field in order to reduce costs of calculation. The same results as those with the full flow-field are obtained. The distances of the planes from the orifice are  $x=0$ ,  $2d$ ,  $4d$ ,  $6d$ ,  $8d$ . The plumes develop from the concave corners of a hexagram orifice rather than from the convex corners. Figure 11 shows velocity vectors right behind the orifice plate. Since a gas tends to discharge in the direction normal to a side of the orifice, the two flows from two sides facing each other run into at the intermediate line and they are merged and pressed out as if the gas flows out from the concave corner. Figure 12 shows the flow directions in a cross section of the symmetric jet at the location  $x=6.5d$ , near the location of the Mach disk. Complicated circulations of flow can be observed in the figure. Figure 13 shows the density contours in various cross sections of jet from an asymmetric orifice. Since the flow from a longer side of the orifice develops stronger than that from a shorter side, the plume is inclined toward the weaker flow. The inclined plume joins to another inclined plume and they grow to a bigger one.

## CONCLUSIONS

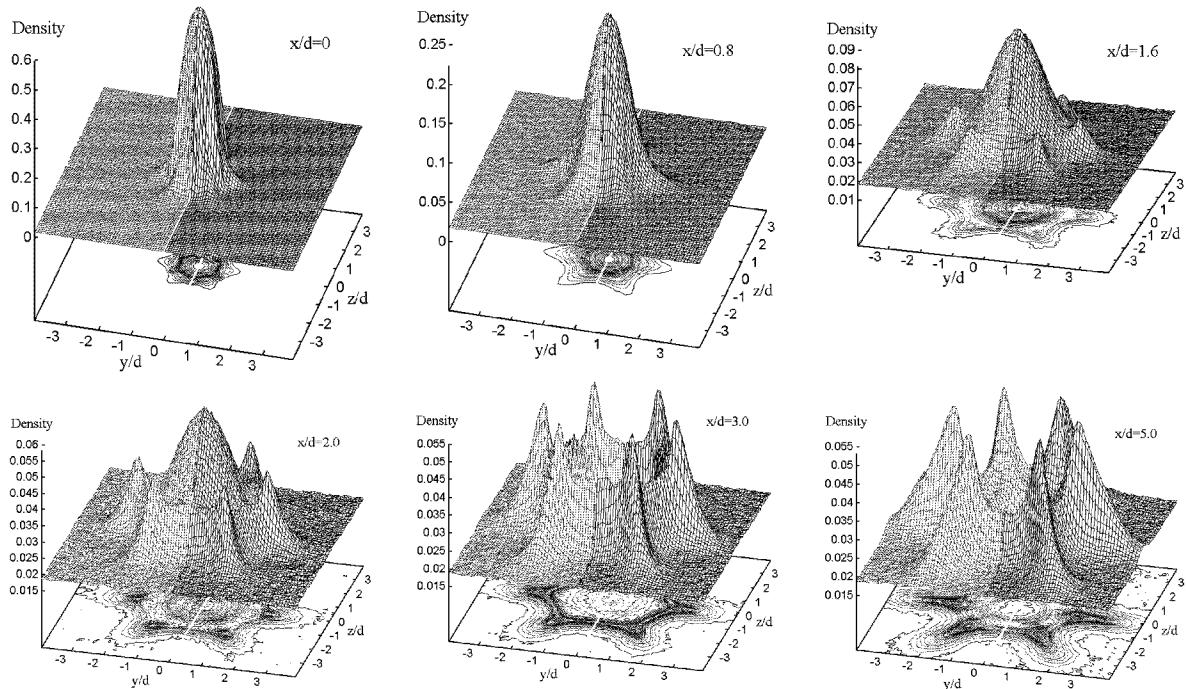
Supersonic free jets from an orifice with convex and concave corners are investigated in three-dimensional field by the DSMC method. The following conclusions have been obtained.

1. The DSMC method is able to simulate the star-shaped jet from an orifice with convex and concave corners, but in the present simulation, due to the roughness of cell network it cannot reproduce the thin jet streams that blow off from the tips of a hexagon.

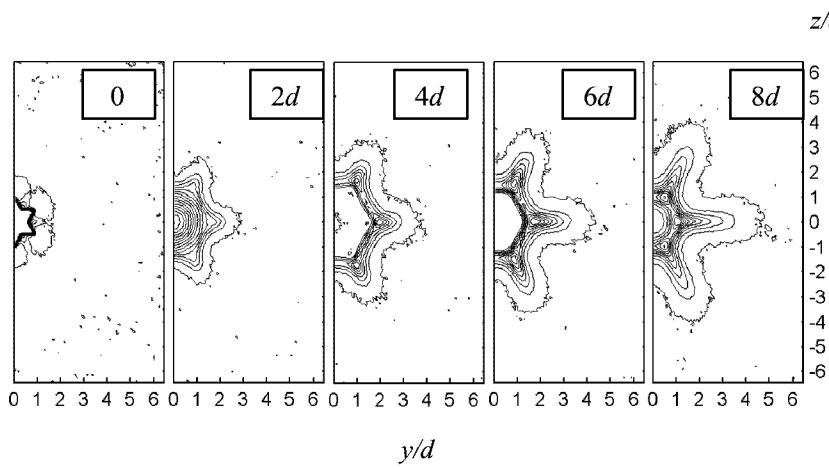


**FIGURE 8.** Mach number profiles, velocity profiles of radial direction, and velocity profiles of tangential direction ( $1/Kn=2500$ ,  $p_0/p_1=100$ )

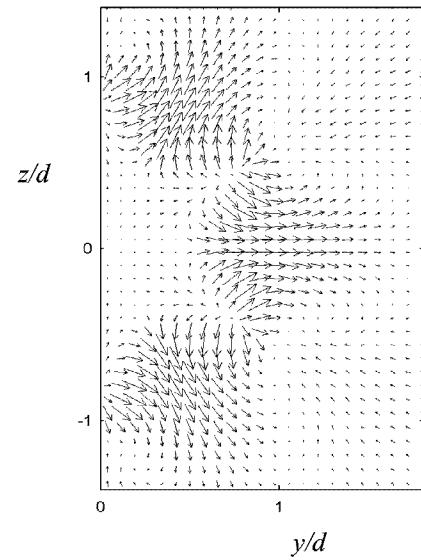
2. The variation of cross section of a star-shaped jet along the jet axis changes with the pressure ratio. The growth of the arms of the star-shaped jet becomes remarkable for  $p_0/p_1=50$  than that for  $p_0/p_1=100$ .
3. The plumes develop faster from the concave corners of a hexagram orifice with symmetric cross section than those from the convex corners. The mechanism of the development is revealed through the observation of velocity vectors right behind the orifice.
4. The directions of flow are also investigated in various cross sections of a jet. There is a complicated flow-field and several circulations of flow are observed.



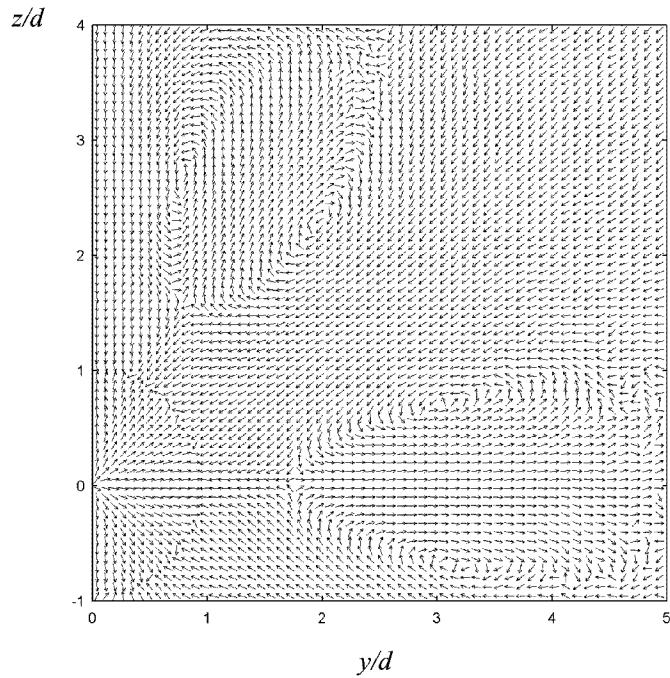
**FIGURE 9.** Density profiles on various planes normal to the jet axis ( $1/Kn=2500$ ,  $p_0/p_1=50$ ).



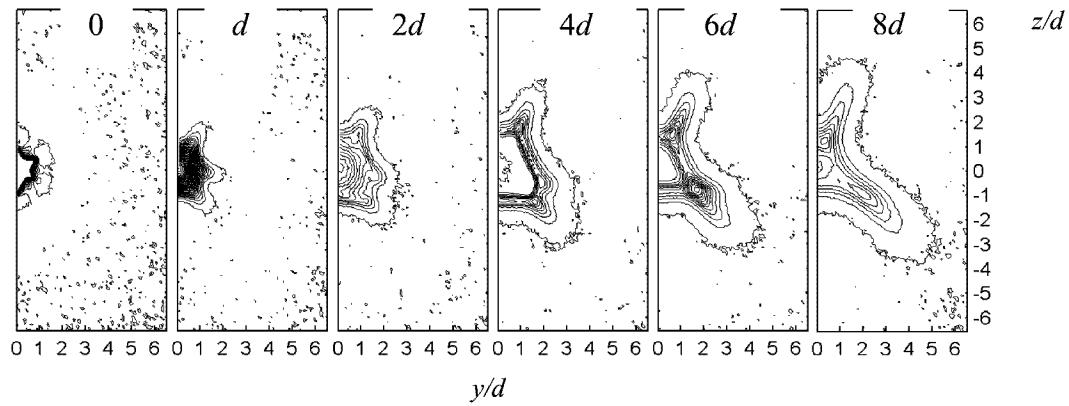
**FIGURE 10.**  
Density contours in planes normal to the axis of jet from the orifice (a).  
( $1/Kn=2500$ ,  $p_0/p_1=50$ ).



**FIGURE 11.** Velocity vectors right behind the orifice (a).



**FIGURE 12.** Flow directions in a cross section of jet near the location of Mach disk.



**FIGURE 13.** Density contours in planes normal to the axis of jet from the orifice (b).

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